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A systematic approach to identifying key parameters and processes in agroecosystem models

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Abstract

Process-based agroecosystem biogeochemistry models are widely used to quantify the flow of water and nutrients in agricultural ecosystems and they have become important tools in the effort to address the twin challenges of reducing greenhouse gas emissions and improving agricultural sustainability. Model parameters require careful calibration, as they affect the simulated processes and outputs. Sensitivity analysis (SA) is commonly used to quantify the impacts of parameters on outputs, and guide the calibration process. Here we demonstrate a systematic approach for SA, which assures that (1) the role of time-dependency in the sensitivity indices is considered and (2) the SA is not biased by the edapho-climatic conditions at individual sites. Demonstrating this approach, we examine the parametric sensitivity of an advanced agroecosystem model (Landscape-DNDC) using a framework that is based on (1) the Sobol SA method, (2) model simulations at three UK arable sites and (3) the grouping of the model's parameters according to the processes they affect. The findings of this research identify the parameters and processes that should be carefully examined in order to minimise the impact of parametric uncertainty on model outputs. We show that a limited

number of parameters are responsible for a large part of the sensitivity of model outputs. The description of soil microbial dynamics is identified as a key source of output sensitivity. Also, we show that individual management activities can significantly affect the time-dependency of the parametric sensitivity indices for certain model outputs.
Keywords: soil biogeochemistry, ecosystem modelling, Landscape-DNDC, sensitivity analysis

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Highlights

- The parametric sensitivity of the Landscape-DNDC agroecosystem biogeochemistry model is quantified.
- 23% of the model's biogeochemistry parameters are responsible for 87% of output sensitivity
- The temporal scale of the analysis is shown to affect the relative importance of the parameters.
- The parameterisation of the processes that describe soil microbial dynamics is key to model predictions.

1. Introduction

Agroecosystem biogeochemistry (BGC) models are computational tools that simulate the processes that drive the fluxes of nutrients through agricultural ecosystems, their interactions and their environmental sensitivity. They take measurable information on the drivers and initial state of the ecosystem (e.g. climate, vegetation type, soil properties etc) and feed them to a set of mathematically-described interacting processes that represent the system and its evolution. Measured input data typically contain uncertainties while the modelled processes can be highly customisable especially if they depend on several parameters. As a consequence, model outputs encapsulate the effects of data and model-related uncertainties. These uncertainties are caused by (1) the spatial and temporal variability of the measured input data (2) the model's structure/architecture and (3) the lack of "precise" quantification of the mathematical and/or statistical parameters that make up the model's formulation. These three uncertainty sources are also known as input, structural and parametric respectively, and they have a combined impact on the model's predictive quality (Campolongo et al., 2007; Norton, 2015; Baroni and Tarantola, 2014).

Analyses of the sensitivities of model outputs to input, structural and parametric uncertainties form an important part of model development and application (Della Peruta et al., 2014; Qin et al., 2016; Fan et al., 2016). SA can be used in model development as a way to simplify a model (i.e. identify less significant parameters/processes) and refine the prior ranges of its parameters (Heinen, 2006). Model users apply SA to identify which parameters to include in model calibration and to gain an understanding of the model's behaviour under the conditions that are specific to their work. Sensitivity analysis of model outputs to model inputs is used to derive estimates of the impacts that the spatiotemporal variability of measurable inputs (e.g. data on climate, soil properties) can have on a model's outputs (Van Oijen et al., 2005; Rafique et al., 2015; van Oijen et al., 2011). The existence of persistent bias in a model's outputs can be controlled by identifying how the architecture of a model's mechanisms, and the mechanisms themselves, affect the model's outputs. The quantification of structural uncertainty can be achieved by evaluating a model under different architectures and module combinations (Sándor et al., 2016; Ruane et al., 2016). Nevertheless, such an exercise requires models that can accomodate a set of conceptually different but interoperable modules and is, thus, more difficult to examine. On the other hand, the quantification of the sensitivities of different outputs to a model's parameters (i.e. parametric sensitivity) is mainly dependent on whether the model's format offers access to its parameters. In this study, we focus exclusively on parametric sensitivity analysis, to which we hereafter refer when using the term *sensitivity analysis* (SA).

Global parametric SA (GSA) methods are commonly used in studies with agroecosystem models. In order to achieve their aim, the values of all the examined parameters are perturbed concurrently and the impact of each parameter (i.e. direct and indirect) on the output of interest is quantified (Pianosi et al., 2016; Norton, 2015; Cariboni et al., 2007). Morris and Sobol are two of the most widely used GSA methods with Sobol being more computationally expensive and detailed than Morris (Confalonieri et al., 2010; Sarrazin et al., 2016; Wainwright et al., 2014; Iooss and Lemaître, 2014; Campolongo et al., 2004). The parametric sensitivity of a model output can be quantified through SA by using (1) a single value (e.g. simulated soil CO_2 at day d); (2) the mean value during a defined period (e.g. annual or weekly mean) or (3) a cumulative amount during a defined period (e.g. cumulative soil CO_2 fluxes during one year). The use of a single simulated data point (e.g. CO_2 flux at day d) to quantify the parametric sensitivity of an output (e.g. CO_2) might not be appropriate for model outputs that behave in a highly dynamic manner (e.g. greenhouse gases). On the other hand, the use of cumulative values for a single time period (e.g. a year, week or month) might not capture all the possible effects of parametric uncertainty on a simulated variable if this variable is highly dependent on other actions. For example, soil N_2O fluxes might be strongly dependent on the timing of fertiliser application just like NO_3 loss through leaching might be dependent on the timing of heavy rainfall events (Gerber et al., 2016; Molina-Herrera et al., 2016; Castellano et al., 2010; Ma et al., 2010). In spite of that, the issue of time-dependency of the estimated sensitivity indices (SI) is rarely examined in SAs with ecosystem BGC models but has been considered in some studies with hydrological models (Song et al., 2013; Pianosi and Wagener, 2015; Guse et al., 2016).

Another important aspect, which is also rarely considered in relevant studies, is the heterogeneity of agroecosystems. Most studies on the parametric sensitivity of agroecosystem models use simulations at a single site to quantify the sensitivity of the model's outputs (Necpálová et al., 2015; Della Peruta et al., 2014; Qin et al., 2016, 2013). However, this approach does not account for the fact that the edapho-climatic conditions at the simulated site could be strongly influencing the estimated SIs and the SA overall (Li et al., 2004). In this respect, the performance of simulations at more than one site is a way to ensure the robustness of the SA. This is important particularly if the model's intended spatial scale of application is large (e.g sub-national level). In general, a lack of studies using process-based agroecosystem BGC models and focusing on the parametric sensitivity of their outputs can been observed in the relevant literature. Most SA studies with agroecosystem BGC models focus on input uncertainty and only few studies have focused on the parametric sensitivity of the models (Qin et al., 2013; Wang and Chen, 2012; Del Grosso et al., 2010; Hastings et al., 2010; Zaehle et al., 2005; Klatt et al., 2016). The role of parametric uncertainty is more often considered in studies that deal with the calibration of model parameters and in which the results of parametric SAs are not always presented or discussed (van Oijen et al., 2011; Lehuger et al., 2009; Rafique et al., 2015; Li et al., 2015). Also, such studies tend to focus only on a single model output (e.g. soil N_2O emissions or soil C content) (Lehuger et al., 2009). In this context, the consideration of more than one model outputs in SAs can provide a more complete picture of how parameters affect model prediction.

In this study, we present a simple framework for the quantification of model parametric sensitivity that is tailored to agroecosystem models. The model that we use to demonstrate the framework is Landscape-DNDC, which is a typical process-based agroecosystem BGC model (Haas et al., 2012). Landscape-DNDC shares similarities with other agroecosystem models in terms of concept, mathematical formulation and parameterisation and more so with other DNDC-based models (Gilhespy et al., 2014; Abdalla et al., 2010; Smith et al., 2010). Therefore, we believe that the results of this study will be relevant to other agroecosystem models. The study focuses on the soil biogeochemistry aspect of the model and our SA examines the importance of the relevant parameters only (i.e. plant growth-related parameters not considered). We use the Sobol SA method (Campolongo et al. (2007)) and collect model outputs for 10 key variables. Taking into account the aforementioned limitations of other SA studies, here, we consider the role of edapho-climatic conditions by performing simulations at three UK arable sites (representative of UK's soils and climate). In order to examine the time-dependency of the estimated sensitivity indices, we collect model outputs at eight different temporal resolutions (i.e. one annual value and seven weekly values). Also, we are interested in understanding the role of processes for model outputs since this can lead to observations that are of practical value in a broader sense.

To examine this aspect, we sort the model's parameters into three groups according to the type and role of the processes that they affect, and examine the contribution of each group to output sensitivity. In summary, the main objectives of the study are to (1) quantify the parametric sensitivity of key outputs of the Landscape-DNDC model; (2) examine how parameter groups affect model outputs and (3) assess the impact of the temporal resolution of the SA on the estimated parametric sensitivities.

2. Materials and methods

2.1. The Sobol method

The Sobol SA method is a global, variance-based and model independent method that can be used to quantify the sensitivity of model outputs to inputs and parameters (Baroni and Tarantola, 2014). The method estimates the first order sensitivity index (S_i), which presents the direct contribution of a parameter (X_i) to an output (Y), and the total sensitivity index (S_T), which represents the direct and indirect contribution of parameter X_i to the sensitivity of Y. (S_i) and (S_T) are estimated using (1) and (2) respectively:

$$S_i = \frac{V\left[E\left(Y|Xi\right)\right]}{V\left(Y\right)} \tag{1}$$

$$S_T = \frac{E\left[V\left(Y|X_{-i}\right)\right]}{V\left(y\right)} \tag{2}$$

where X_{-i} denotes all inputs except X_i, V denotes the variance and E the expectation. The Sobol method also allows for the estimation of sensivity indices of higher order (i.e. second, third etc). For example, the second order Sobol sensitiviy index S_{ij} quantifies the variance caused to Y by the interaction between parameters X_i and X_j. The number of model simulations (R) that is required for the estimation of S_i and S_T is equal to $N(2D+2)$ where N is the sample size and D is the number of parameters (Nossent et al., 2011). The value of N is case-specific with values in the relevant literature ranging between a few hundred and tens of thousands (Nossent et al., 2011; Wainwright et al., 2014; Pianosi and Wagener, 2015). The examination of the convergence of the estimated SIs can be used to ensure that the chosen N was sufficiently large (Sarrazin et al., 2016). In this study, the convergence of the estimated SIs, as it was reflected in the respective confidence intervals, was assessed visually and was achieved by setting N equal to 5000 (i.e. R=1.24 million).

2.2. Landscape-DNDC

Landscape-DNDC (hereafter referred to as *the model*) is a process-based ecosystem model that describes the biogeochemistry of terrestrial ecosystems. Most of the model's description of biogeochemical processes comes from the original DeNitrification-DeCompositon model (DNDC) (Li et al., 1992). However, it is even more closely related, in terms of concept, structure and mathematical formulation, to the mobile-DNDC model(Chirinda et al., 2010). The model can simulate energy fluxes, and water and nutrient transport inside the soil-plant-atmosphere system at arable, grassland and forest ecosystems. It has a modular structure that facilitates the integration of modules, which describe different part of the simulated system (i.e. plant growth, water cycling, soil BGC and microclimatic conditions). It is a transparent model, in the sense that the user has access to the parameters of the model's modules, while the user can also reshape the model's structure and use different module combinations. The model requires input data on climatic (e.g. min/max precipitation, temperature, wind speed) and soil (e.g ph, clay content, bulk density) conditions as well as information on field management (e.g. crop rotation, date/depth of tillage) (Haas et al., 2012).

The model simulates the interconnected soil biogeochemical processes on a daily basis. The properties of the simulated soil can change with depth according to user-defined information (e.g. number of soil layers, layer thickness etc) and all soil-related model calculations are performed on a layer-by-layer basis. The total carbon (C) content of the ecosystem is stored in (1) the growing plant's parts and (2) the soil's C pool (Fig. 1). The soil's total C is allocated into three pools, which differ in terms of activeness (i.e. fast/slow C decomposition) and are interconnected. The soil's living organisms (i.e. microbes) are conceptually considered as a part of the soil's total C. The microbe-mediated decomposition of C in the pools (decomposers are named humads in Landscape-DNDC) is the main driver of change in the soil's C budget and it is also a source of CO_2. The nitrogen (N) content of the plant-soil system, and of its different compartments, has a controlling role over the movement of C between the different C pools.

The model's N pools (N_2, N_2O, NO, NO_2, clay-bound NH_4, NO_3, unbound NH_4 and urea) are mainly controlled by the input of organic (manure) and mineral (ammonium nitrate) N (Fig. 1). The daily budget of N in the pools changes as a result of the processes of N addition, N plant uptake, N leaching, N mineralisation/immobilisation, nitrification/denitrification and ammonia (NH_3) volatilisation. Nitrogen-based gas production in the soil is

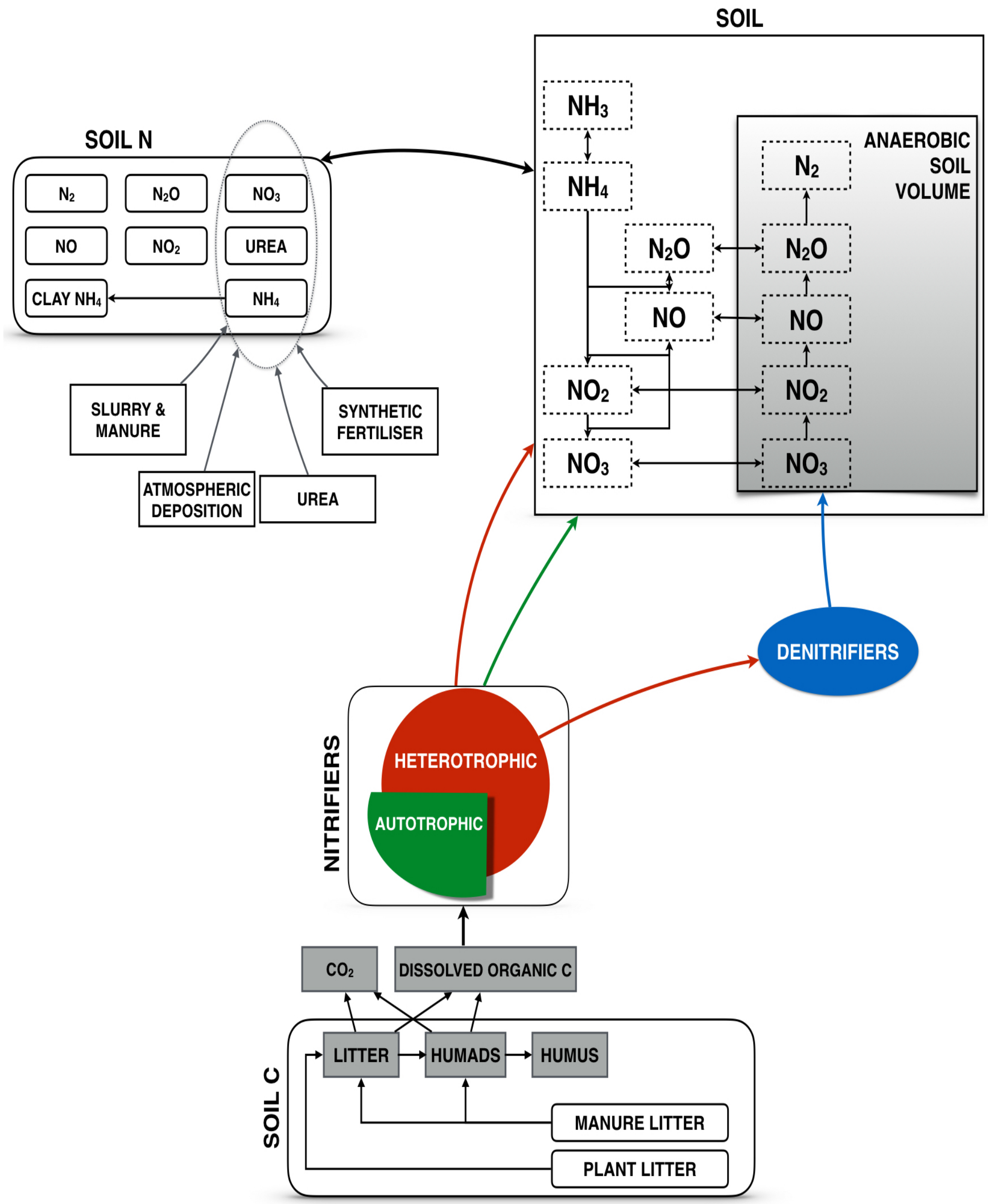

Figure 1: Schematic description of the main processes controlling carbon and nitrogen cycling in the soil as simulated in the Landscape-DNDC model.

the result of nitrification and nitrification. These processes are affected by the soil's hydrological conditions as well as its temperature, ph and other physical properties (e.g. bulk density). Any addition of N to the soil system (via fertiliser application, plant parts etc) affects the web of interacting N-related processes. After a certain amount of N is added to the soil, it will flow through the web of processes and reach one (or more) of the possible endpoints (e.g. become N gas, get leached to groundwater etc). The relative size of each N pool along with the soil's physical, biochemical, hydrologic and microclimatic conditions at each simulated day, will collectively affect how much N reaches each endpoint as well as how fast this will happen.

The model's soil BGC module uses a total of 123 parameters to simulate the soil's biogeochemical processes in agricultural soils. For each parameter, a default value and a range of possible values (i.e. minimum and maximum) are provided. Due to the number of parameters involved in the mathematical representation of the modelled processes and the complexity of their interactions, the relationships between parameters and outputs are non-monotonic and the model is non-linear (Rahn et al., 2012). The model does not allow the use of values that are outside the predefined ranges and, therefore, we use the recommended parameter ranges to define the upper and lower bounds in the SA sampling process. In order to facilitate the presentation of the SA results and make them easier to understand the model's BGC parameters have been classified into 3 groups of parameters based on their relative role and position within the model's mathematical structure:

1. The first group includes all the parameters that directly control the population and dynamics of soil microbes. This group also contains

the parameters that directly control the size and dynamics of the different soil C pools because (1) microbes themselves are conceptually considered part of the soil's C and (2) microbial growth/death processes are tightly coupled to soil C dynamics. We use the acronym MPD (for Microbial Population and Dynamics) when referring to this group of parameters.

2. The second group of parameters contains all the parameters that directly control the production and subsequent diffusion of N and C-based gases from the soil. We use the acronym GPD (for Gas Production and Diffusion) when referring to this group of parameters.

3. The third group, contains all the parameters that link the soil's physical and chemical condition (e.g. pH, temperature, moisture) to microbial activity, soil C dynamics and gas production and diffusion. We use the acronym EC (for Edapho-Climatic) when referring to this group of parameters.

Tables 1, 2 and 3 present the parameter groups and provide details on the parameters contained in each group. Further details about the model, its structure, processes and parameters can be found in Butterbach-Bahl et al. (2015)

Table 1: Landscape-DNDC parameters that belong to the MPD group of parameters

Name	Lower Boundary	Upper Boundary	Description
AMAXX	0.9817	1.6362	Microbial death rate
DENIFRAC	0.525	0.875	Microbial denitrifier fraction
EFFAC	0.525	0.875	Fraction of decomposed carbon that goes to the dissolved organic carbon pool
FDL	0.375	0.625	Fraction of decomposed labile litter that is assimilated by microbes instantaniously
FDR	0.2625	0.4375	Fraction of decomposed recalcitrant litter that is assimilated by microbes instantaniously
FDVL	0.4875	0.8125	Fraction of decomposed very labile litter that is assimilated by microbes instantaniously
FNO_3 U	0.5625	0.9	Factor steering NO3 availability for microbial assimilation
FRC	0.0375	0.0625	Factor accounting for litter availability dependency on microbial death
KCRB L	0.06937	0.11563	Decomposition constant for labile inactive microbes
KCRB R	0.00167	0.00278	Decomposition constant for recalcitrant inactive microbes
KHDC L	0.00055	0.00093	Decomposition constant for labile humads
KHDC R	0.000277	0.000463	Decomposition constant for recalcitrant humads
KICE	0.5625	0.9375	Ice dependency on effective diffusion coefficient
KLRAW	0.0375	0.0625	Decomposition constant for raw litter
KRCH	2.8e-06	4.6e-06	Decomposition rate for humus pool
KRCL	0.01387	0.02312	Decomposition rate for labile carbon pool
KRCR	0.0056	0.0093	Decomposition rate for recalcitrant carbon pool
KRCVL	0.0694	0.1156	Decomposition rate for very labile carbon pool
MICRRESP	0.06	0.1	Factor determining microbial respiration
MN_2O	0.0592	0.0988	Microbial maintenance coefficient for denitrification of N_2O
MNO_2	0.0263	0.0438	Microbial maintenance coefficient for denitrification of NO_2
MNO_3	0.0675	0.1125	Microbial maintenance coefficient for denitrification of NO_3
MNO	0.0592	0.0988	Microbial maintenance coefficient for denitrification of NO
MUEMAX	3.6547	6.0913	Microbial growth rate
MUE N_2O	0.255	0.425	Microbial growth rate for denitrification on N_2O
MUE NO_2	0.5025	0.8375	Microbial growth rate for denitrification on NO_2
MUE NO_3	0.5025	0.8375	Microbial growth rate for denitrification on NO_3
MUE NO	0.255	0.425	Microbial growth rate for denitrification on NO
PERTL	0.00038	0.00063	Downward transport of labile litter
PERTMAX	0.225	0.375	Limit depth for litter transport
PERTR	8e-05	0.00013	Downward transport of recalcitrant litter.
PERTVL	0.0075	0.0125	Downward transport of very labile litter
RBO	0.15	0.25	Fraction of inactive microbes in active organic material pool
RCEC	34.5	57.5	Factor determining CO_2 production during decomposition
RCNB	6.0	10.0	C:N ratio of inactive microbes in active organic material pool
RCNH	9.0	15.0	C:N ratio of humads in active organic material pool
RCNM	7.35	12.25	C:N ratio of humus
RCNRR	180.0	300.0	C:N ratio of resistant residues
RCNRVL	18.0	30.0	C:N ratio of very labile residues
SHR	0.12	0.2	Fraction of labile humads
SRB	0.675	0.99	Fraction of labile inactive microbes

Table 2: Landscape-DNDC parameters that belong to the GPD group of parameters

Name	Lower Boundary	Upper Boundary	Description
DIFF C	0.1875	0.3125	Diffusion constant for carbon compounds between aerobic an anaerobic microsites
DIFF N	0.375	0.625	Diffusion constant for nitrogen compounds between aerobic an anaerobic microsites
DNDC KMM C DENIT	0.0128	0.0213	Michaelis-menten constant for carbon dependency of denitrification
DNDC KMM C MIC	0.0039	0.0066	Michaelis-menten constant for carbon dependency of microbial growth
DNDC KMM NH_4 NIT	6.63e-05	0.0001105	Michaelis-menten constant for NH_4 dependency of nitrification
DNDC KMM NO_2 NIT	1.88e-06	3.13e-06	Michaelis-menten constant for NO_2 dependency of nitrification
DNDC KMM NO_3 TRANSNH_4	8e-05	0.00013	Michaelis-menten constant for nitrogen dependency of dissimilatory nitrate reduction to ammonium
DNDC KMM N DENIT	0.0622	0.1038	Michaelis-menten constant for nitrogen dependency of denitrification.
DNDC KMM N MIC	0.0014	0.0024	Michaelis-menten constant for nitrogen dependency of microbial growth
DNDC KMM O_2 DECOMP	0.225	0.375	Michaelis-menten constant for O2 dependency of decomposition.
D N_2O	0.0465	0.0775	Reduction constant for N_2O diffusion
D NO	0.0547	0.0912	Reduction constant for NO diffusion
EFF N_2O	0.0562	0.0938	Microbial efficiency for N_2O denitrification
EFF NO_2	0.321	0.535	Microbial efficiency for NO_2 denitrification
EFF NO_3	0.3008	0.5012	Microbial efficiency for NO_3 denitrification
EFF NO	0.1132	0.1888	Microbial efficiency for NO denitrification
FCO_2 1	0.9075	1.5125	Factor for CO_2 production during humads decomposition process
FCO_2 2	1.68	2.8	Factor for CO_2 production during humads decomposition process
FCO_2 3	1.725	2.875	Factor for CO_2 production during humads decomposition process
FCO_2 4	0.0638	0.1063	Factor for CO_2 production during humads decomposition process
FCO_2 HU	0.6	1.0	Factor for CO_2 production during humads decomposition process
FTRANS	0.0037	0.0063	Factor steering dissimilatory nitrate reduction to ammonium
KCHEM	6.0	10.0	Reaction rate for chemo-denitrification
KN_2O	0.0037	0.0063	Reaction rate for N_2O reductase
KNIT	0.75	1.25	Reaction rate for nitrification
KNO	0.0015	0.0025	Reaction rate for NO reductase
NH_4 DENIMAX	0.6	1.0	Maximum nitrification fraction of NH4
RCEC	34.5	57.5	Factor determining CO_2 production during decomposition

2.3. Model outputs

As part of the sensitivity analyses, at each model evaluation instance, we collect model outputs for 10 variables, which are presented in Table 4. In order to examine the sensitivity of each model output to the model's parameters at selected timeframes, at the end of each model evaluation, we collect (1) the annual sum for each variable (e.g. amount of N_2O emitted during a whole year) and (2) seven weekly subsets (e.g. weekly cumulative soil N_2O flux). The seven weekly subsets of outputs are the sum of the daily outputs during each of the seven weeks. For each site, the first and last day of the seven weeks period has been chosen in such a way as to include all days between a few days before the first date of fertiliser application and a few days after the last date of fertiliser application. Agricultural soils remain in relative biogeochemical stability when no crop is cultivated and no fertiliser is added. Under crop growing conditions, the input of fertiliser to the soil system is the most important trigger of biogeochemical activity. Therefore, the parametric sensitivity of outputs, and especially those strongly related to fertiliser use, can be temporally dynamic. Through the use of the seven weekly sums for each site the impact of fertiliser addition to the soil is integrated in the SA process. The annual outputs' sums are used in the SA to provide a picture of the parametric sensitivities of outputs on an annual basis while the seven weekly outputs' subsets to provide snapshots that capture the temporal variability of the same parametric sensitivities.

2.4. Experimental site data

The model was used to simulate the variables shown in Table 4 at three experimental arable sites which are located in the UK. The experiments have

Table 3: Landscape-DNDC parameters that belong to the EC group of parameters

Name	Lower Boundary	Upper Boundary	Description
EVALIM	0.3	0.5	Maximum depth of soil layer evaporation
EXP1 NX	1.5	2.0	Factor accounting for soil porosity effect on nitrogen effective diffusion coefficient
EXP1 O_2	1.5	2.0	Factor accounting for soil porosity effect on oxygen effective diffusion coefficient
EXP2 NX	1.5	1.875	Factor accounting for soil porosity effect on nitrogen effective diffusion coefficient
EXP2 O_2	0.9375	1.5625	Factor accounting for soil porosity effect on oxygen effective diffusion coefficient
FCLAY1	0.105	0.175	Factor for clay dependency of humads decomposition process
FCLAY2	1.7269	2.8782	Factor for clay dependency of humads decomposition process
FPERCOL	0.675	0.9	Fraction of surface water that goes into runoff
FRUNOFF	0.1875	0.3125	Fraction of daily runoff from surface water
MCOEFF	0.0011	0.0019	Maximum snow melting rate
MELTMAX	1.875	3.125	Maximum melted ice fraction per day
M FACT DEC1	0.4462	0.7437	Factor determining dependency of decomposition on water filled pore space
M FACT DEC2	6.0	10.0	Factor determining dependency of decomposition on water filled pore space
M FACT P1	0.3375	0.5625	Factor determining dependency of nitrification on water filled pore space
M FACT P2	30.0	50.0	Factor determining dependency of nitrification on water filled pore space
M FACT P3	0.4125	0.6875	Factor determining dependency of N2O production during nitrification on water filled pore space.
M FACT P4	3.75	6.25	Factor determining dependency of N2O production during nitrification on water filled pore space
M FACT P5	0.1688	0.2813	Factor determining dependency of microbial activity on water filled pore space
M FACT P6	7.5	12.5	Factor determining dependency of microbial activity on water filled pore space
PHCRIT N_2O	3.75	6.25	Factor for pH dependency of N_2O denitrification
PHCRIT NO_2	4.575	7.625	Factor for pH dependency of NO_2 denitrification
PHCRIT NO_3	4.725	7.875	Factor for pH dependency of NO_3 denitrification
PHDELTA N_2O	0.4612	0.7688	Factor for pH dependency of N_2O denitrification
PHDELTA NO_2	1.08	1.8	Factor for pH dependency of NO_2 denitrification
PHDELTA NO_3	1.14	1.9	Factor for pH dependency of NO_3 denitrification
PHMAX	7.5	12.5	Maximum allowed pH value
PHMIN	1.875	3.125	Minimum allowed pH value
PHMIN CHEM	3.75	6.25	Factor for pH dependency of chemodenitrification
PHOPT CHEM	0.45	0.75	Factor for pH dependency of chemodenitrification
PH FACT P2	0.975	1.625	Factor for pH dependency of nitrification
PH FACT P3	0.06	0.1	Factor for pH dependency of nitrification
PH FACT P4	0.75	1.25	Factor for pH dependency of N2O production during nitrification
PH FACT P5	2.8125	4.6875	Factor for pH dependency of chemodenitrification
PSL SC	0.015	0.025	Empirical decrease of hydraulic conductivity of coarse discretized soil layers
PSL WC	0.015	0.025	Base layer depth for evaporation decrease with depth
PT ALPHA	0.825	1.375	Priestley-Taylor coefficient of advection
RCLAY	0.225	0.375	Factor determining clay dependency of soil water evaporation
SLOPE CLAYF	0.05	0.08	Factor determining clay dependency of soil water evaporation
SLOPE FF	0.75	1.25	Specific slope factor for water flux from litter layers
SLOPE MS	2.0	3.0	Specific slope factor for water flux from mineral soil
TEXP	1.293	2.155	Temperature dependency of diffusion between aerobic and anaerobic soil
TF CHEM1	0.075	0.125	Temperature dependency of chemodenitrification
TF CHEM2	0.0975	0.1625	Temperature dependency of chemodenitrification
TF DEC1	2.655	4.425	Temperature dependency of decomposition
TF DEC2	27.75	46.25	Temperature dependency of decomposition
TF DEN1	3.0	5.0	Temperature dependency of denitrification
TF DEN2	30.0	50.0	Temperature dependency of denitrification
TF NUP N2O1	0.04133	0.06888	Temperature dependency of N_2O production during nitrification
TF NUP N2O2	7.0575	11.7625	Temperature dependency of N_2O production during nitrification
TF NUP NO1	0.017813	0.029687	Temperature dependency of NO production during nitrification
TF NUP NO2	6.675	11.125	Temperature dependency of NO production during nitrification
TREF	33.75	56.25	Reference temperature for NH_3 volatilization

Table 4: Model outputs

Variable	Description	Unit
N_2O	Nitrous oxide gas	kgN/ha
NO	Nitric oxide gas	kgN/ha
N_2	Nitrogen gas	kgN/ha
NO_3	Nitrate leaching	kgN/ha
NH_3	Ammonia gas	kgN/ha
N Uptake	Nitrogen uptake gas	kgN/ha
Soil C	Soil carbon	kgC/ha
Microbial population	Soil microbial biomass	kgC/ha
Nitrification	Nitrification rate	kgN/ha
Mineralisation	Nitrogen mineralisation rate	kgN/ha

taken place in 2011 at two of the sites and in 2010 at the third one. Table 5 presents information about the soil, management and climatic conditions at the three experimental site.

3. Results

3.1. Results on annual basis

The estimated S_Ts for each site and variable showed that only few parameters had a noticeable effect on the examined model outputs (see Appendix for detailed results). Based on these results, we can be confident that the most important model parameters have been identified and that the edapho-climatic conditions have not affected the ranking of the most important parameters relative to the examined outputs.

In order to present how the three groups of parameters (i.e. MPD, GPD and EC) affect the examined model outputs we extracted, for each site and

Table 5: Experimental sites information

	Terrington	**Edinburgh**	**Gleadthorpe**
Latitude/Longitude	52.75/0.3	55.86/-3.2	53.21/-1.07
Year	2011	2011	2010
Crop	Winter Wheat	Spring Barley	Spring Barley
N applied (kg/ha)	280	144	130
Julian day(s) of N application	75/94/108	100/144	81/110
N applied per application (kgN/ha)	60/110/110	40/104	40/90
Bulk Density	1.34	1.26	1.43
Texture	Sandy Loam	Clay Loam	Sandy Loam
Clay (%)	11	34	11
Soil C (%)	1.8	4.9	1.6
pH	8.3	6.7	6.0
Annual precipitation (mm)	472	1312	888
Mean temperature (^{o}C)	12	9	9

output variable, the 20 most important parameters (i.e. 20 highest S_is). The fact that (i) the ranking of the parameters relative to each variable was the same across all sites and that (ii) S_i quantifies the parameter-induced variance of an output allowed us to calculate the mean S_i for each output-site combination. This was done in order to merge the information produced by the SA for each site into a single set of S_is per output. In this way, the effects of the variation in edapho-climatic conditions across the three sites were integrated into each estimated mean S_i. In this context, by "sensitivity of output Y" we, hereafter, refer to the mean S_i of Y that was estimated for the three experimental sites. Based on this, the 28 parameters with the highest S_i caused, on average, 87% of output sensitivity. While the magnitudes of the estimated S_Ts vary between sites the relative importance of the parameters (i.e. their ranking) does not. Figure 2 presents 10 pie charts (one for each model output) that show the contribution of each group of parameters to the variation in the respective model output. These results show that the GPD group of parameters has a noticeable contribution to the sensitivity of simulated emissions of gases (N_2O, NO, N_2, NH_3) in contrast to a minor contribution to that of the rest of the outputs. Surprisingly, the parameters related to gas production and diffusion (GPD group) also play a noticeable role in the sensitivity of NO_3 prediction. The EC and MPD groups of parameters have significant contribution to all model ouputs. EC parameters appear to be particularly important for NH_3, NO_3, soil C and N uptake while MPD parameters appear to be most important for microbial population, mineralisation and nitrification.

To supplement Figure 2 and look into the role individual parameters we collected those parameters that were found to be important relevant to each of the examined outputs (i.e. 28 highest ranked parameters). We then quantified their relative contribution (%) to the sensitivity of each output. In order to quantify the total parametric sensitivity of an output we used the sum of all estimated S_is for that output (i.e. mean Si across the three sites). Figure 3 presents the most important model parameters per parameter group and their relative contribution to the sensitivity of the 10 examined model outputs.

3.1.1. N-based gases

The N_2O, NO, N_2 and NH_3 charts in Figure 2 show that most of the variation that is caused to the simulated emissions of N-based gases is due to the MPD and EC parameters. This is expectable not only because these

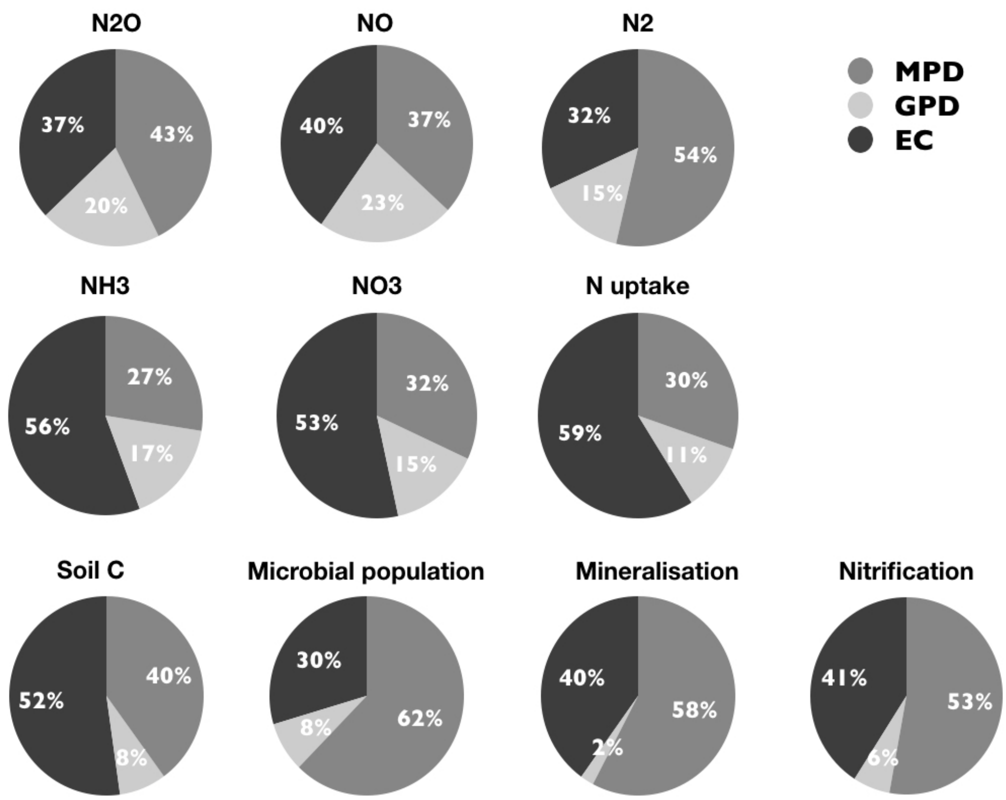

Figure 2: Contribution of each parameter group to the sensitivity of the examined model outputs

two groups, when combined, make up the majority of the model's parameters but also because they affect the size and state of the N-based soil substrate. In this context, it should be noted that fewer parameters are included in the GPD group compared to the MPD and EC groups. Taking this fact into account, the noticeable contribution of the GPD group of parameters to the sensitivity of simulated N-gases (ie. on average 19%) is reflective of the importance of those model parameters that directly control the processes of gas production and diffusion. The parameters that make up the GPD group vary between the different types of gases and no individual parameter stands out as being of noticeable importance. The only exception is the dominant role of the parameter that defines the gross rate of nitrification (i.e. KNIT) in relation to the prediction of NH_3 volatilisation; where it caused around 70% of the total GPD-induced sensitivity of the simulated NH_3.

In terms of the MPD group of parameters, its contribution is mainly due to the impact of 3 parameters: (1) the microbial death rate parameter (AMAXX) which controls the amount of soil microbes; (2) the parameter (EFFAC) that defines the fraction of decomposed C that goes to the dissolved organic C pool which is in turn the life source for the soil's microbes and (3) the parameter (DENIFRAC) that defines how many nitrifying microbes become denitrifiers under anaerobic conditions. The contribution of the EC group of parameters is mainly due to a couple of parameters which relate the soil's temperature (TF DEC) and moisture (M FACT DEC) to decomposition and its pH (PHCRIT) to denitrification. In the case of NH_3 the parameter that directly links the soil's temperature to the volatilisation proneness of NH_3 (TREF) is also a very important role (represented 20% of the total contribution of the EC group to NH_3).

3.1.2. NO_3 leaching

The model's prediction of NO_3 leaching from the soil is to a significant extent affected by the same EC parameters that affect the model's prediction of N-gases. In terms of the MPD group of parameters, EFFAC was found to be the single most important MPD parameter (represented almost half of this group's overall contribution). The GPD group of parameters contributed by 15% to the sensitivity of the simulated NO_3. This share may seem large considering that NO_3 is not a gas but it is explained by the fact that GPD parameters affect not only the diffusion of gases in the soil but also their production. In this context, GPD parameters can indirectly determine the amount of leachable NO_3 by affecting how much is produced via nitrification and lost to the atmosphere via denitrification.

3.1.3. N uptake

The uptake of N by plants is largely influenced (59%) by the values given to the EC parameters. This is mainly due to the simplistic approach that Landscape-DNDC uses to describe plant N update according to which plants have a priority over the soil's N and their ability to take up nutrients and grow can be constrained by the soil's water content (e.g drought conditions). It is therefore easy to see why the parameters that make up the EC group in relation to N uptake included a set of parameters that influence the soil's moisture level (i.e. SLOPE MS, PSL WC, M FACT and RCLAY). Similar to what was seen for the MPD group for NO_3 and the N-based gases, EFFAC was found to be at the top of the list of the most important MPD parameters.

A few parameters that control the turnover of the soil's most active C pools (including the microbial pool) were also among the most important of MPD group. On the other hand, GPD parameters are not strongly related to N uptake and thus had a minor contribution to its sensitivity.

3.1.4. Soil C

EC (52%) and MPD (40%) parameters are almost entirely responsible for the sensitivity of the simulated soil C. The contribution of the EC group is mainly made up by four parameters, of which two are used to link soil moisture conditions to C decomposition (M FACT DEC1 and M FACT DEC2) and two are used to link the soil's temperature to C decomposition (TF DEC1 and TF DEC2). On the other hand, the impact of the MPD group is mainly due to the EFFAC parameter and a few parameters that are related to the turnover of the soil's microbial sub-pools (i.e. RCNH, RBO, KCRB L)

3.1.5. Microbial Population, Nitrification and Mineralisation

The simulation of microbial population is closely associated to the that of nitrification and mineralisation because microbes drive both of these processes. This fact is clearly imprinted in the results of the SA which show very similar patterns with MPD parameters contributing 50-60% of the sensitivity of these outputs and EC contributing most of the remaining part. Similar to what was found for soil C, the EC group is made up by those parameters that relate the soil's moisture and temperature to C decomposition (i.e. M FACT DEC and TF DEC). In the same way, the MPD group is made up by the EFFAC parameter and two parameters that are related to the turnover of the soil's microbial sub-pools (RBO and RCNB). Finally, it was observed that the GPD group of parameters plays a minor role in relation to the simulation of microbial population (8%), nitrification (6%) and mineralisation (2%)

GROUP	PARAMETER	Relative contribution (%) to output sensitivity									
		N_2	N_2O	NO	NH_3	NO_3	N Uptake	Soil C	Microbial Population	Mineralisation	Nitrification
MPD	AMAXX	< 2	3	6	4	3	3	< 2	8	< 2	< 2
	DENIFRAC	< 2	< 2	4	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	EFFAC	19	5	7	6	12	11	14	35	32	24
	KCRB L	4	< 2	< 2	< 2	< 2	2	3	3	2	< 2
	SRB	2	2	< 2	< 2	< 2	< 2	< 2	< 2	3	3
	KRCL	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2	4
	RBO	4	5	< 2	< 2	< 2	< 2	2	3	6	6
	RCNB	4	< 2	< 2	2	2	< 2	< 2	< 2	13	10
	RCNH	4	< 2	< 2	< 2	< 2	< 2	5	< 2	< 2	< 2
	MUEMAX	3	2	5	< 2	< 2	2	< 2	< 2	< 2	< 2
	MUE NO2	< 2	9	4	< 2	< 2	< 2	< 2	< 2	< 2	< 2
GPD	D NO	< 2	< 2	3	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	D N2O	< 2	5	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	DNDC KMM C DENIT	< 2	2	5	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	DNDC KMM N DENIT	4	< 2	3	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	EFF NO2	< 2	4	4	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	KNIT	< 2	< 2	< 2	10	8	3	2	< 2	< 2	< 2
EC	EXP1 NX	< 2	6	6	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	M FACT DEC 1	5	2	10	14	20	21	13	10	24	22
	M FACT DEC 2	3	2	2	< 2	4	< 2	7	4	5	4
	PHCRIT N2O	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	PHCRIT NO2	2	8	< 2	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	PHCRIT NO3	< 2	3	9	< 2	< 2	< 2	< 2	< 2	< 2	< 2
	PSLWC	3	< 2	4	7	7	7	7	< 2	2	2
	SLOPE MS	2	< 2	< 2	5	5	8	< 2	< 2	< 2	< 2
	TF DEC 1	3	< 2	< 2	3	3	< 2	5	2	5	4
	TF DEC 2	3	3	< 2	2	2	7	11	< 2	< 2	3
	TREF	< 2	< 2	< 2	11	4	< 2	< 2	< 2	< 2	< 2
all groups	all other parameters	20	16	12	13	16	14	10	15	6	9

Figure 3: Heatmap of the relative contribution (%) of the 28 most important model parameters to the sensitivity of each output (i.e. the sum of the estimated S_is per output). By "all groups - all other parameters" we refer to the contribution of the remaining 95 model parameters to the sensitivity of an output. All values were rounded before being added to the table.

3.2. Results on weekly basis

Weekly model outputs were used in this study in order to examine the role of the temporal resolution of model outputs to the SA results. This examination is performed by comparing (1) the list of important model parameters (i.e. high S_T) as estimated by the SA when using the weekly-resolution model outputs to (2) the list of important parameters as estimated when using the annual-resolution model outputs. In order to quantify the similarity between weekly and annual-based SA results we use a metric that we name *similarity*. The similarity value is estimated following a 4-step process:

1. For each of the three examined sites and for each of the seven sets of weekly-based SA results we collect the 10 and 50 most important parameters (i.e. highest S_T).

2. For each of the three examined sites we collect the 10 and 50 most important parameters in the annual SA results.

3. We quantify (and express as %) how many of the parameters that appear in the top 10 and 50 annual-based SA results also appear in the respective weekly-based SA results

4. We calculate the average top 10 and top 50 similarity (%) for each variable across all sites

By comparing the similarity of the 50 most important parameters on an annual basis with the 50 the most important parameters on a weekly basis (expressed as the top 50 similarity %) we can identify how many parameters appear as important on a weekly basis but their importance becomes

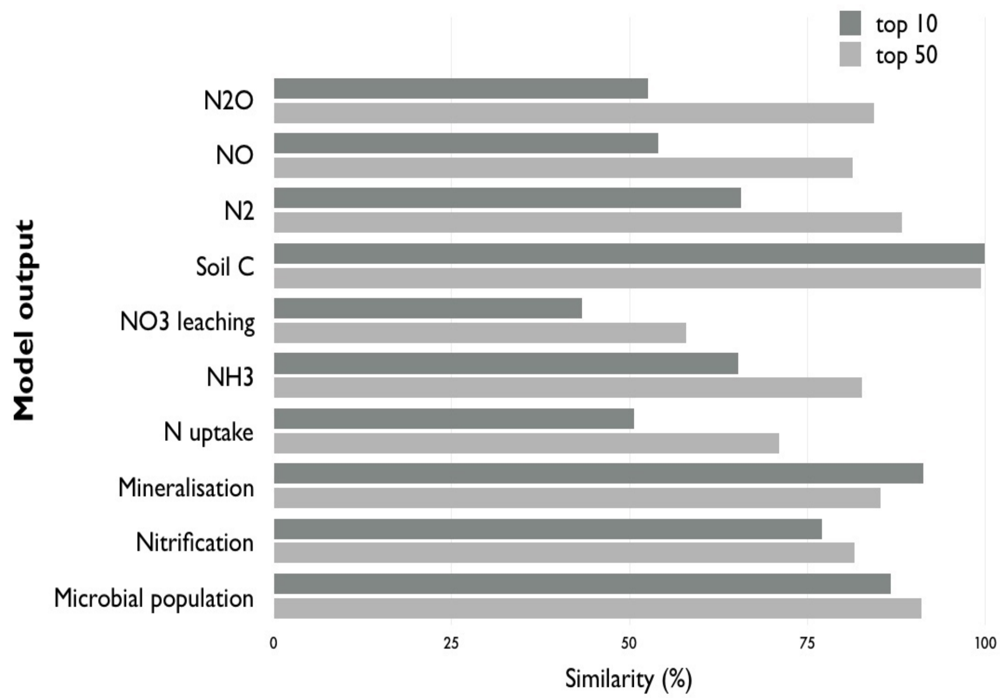

Figure 4: Similarity (%) of the top 10 and the top 50 most important model parameters between the weekly-based and the annual-based SA results

"muted" at an annual basis. The lower the top 50 similarity % is the more the parameters that appear as important only on the weekly-based SA results. In a similar way, by juxtaposing the top 10% similarity values with the top 50 similarity % values we can assess how important is the role of these "muted" parameters during the 7-week period. A large difference (i.e. $> 30\%$) between the top 10 and the top 50 similarity % combined with a low top 50 similarity % suggests that a lot of the "muted" parameters have a higher-than-average ranking; thus important parameters were not captured by the annual-based SA.

The results (Figure 4) suggest that the 50 most important parameters that were identified as such by using the model's outputs at an annual resolution make up around 4/5 of those identified as important when using outputs at a weekly resolution. The picture looks more complex if we look at the top 10 parameters, where roughly 2/3 of the annually-important parameters are found in the weekly-important parameters' lists. On this basis, it can be argued that the relative importance of a considerable number of the high-S_T parameters (of the annually-based SA results) exhibit a temporally dynamic behaviour, which is revealed when examining output sensitivity at a higher temporal resolution (i.e. weeks).

Additionally, the weekly-resolution SA results prove that losing sight of parameters that are important relative to certain outputs when utilising the annual-resolution outputs in the SA, is a possibility. For example, one would have probably concluded that the top 50 (or 10) parameters that came out of the SA analysis using annual-resolution model outputs for NO_3 leaching are, in fact, the 50 (or 10) most important parameters. However, a low similarity of both the top 10 and top 50 parameters for NO_3 leaching suggests that there are almost as many parameters (i.e. 10 and 50) that affect the simulated NO_3 leaching but were not captured by the annual-based SA. This is explained by the fact that NO_3 leaching is strongly influenced by heavy precipitation events. While NO_3 leaching stands out we could also argue that N-based outputs are somehow affected by parameters that become "muted" when we look at the annual-based SA results (more acute for NO_3, NH_3 and N uptake).

4. Discussion

4.1. Parameter groups

The results of this study showed that the parameterisation of the processes that describe the growth and death of soil microbes play significant role in how the model simulates the examined variables. The MPD group of parameters is particularly important in the simulation of the soil's microbial population and of the associated processes of mineralisation and nitrification. Moreover, MPD parameters were proven to be important in terms of the model's prediction of N_2O, N_2 and NO_3 leaching. Soil N_2O fluxes and NO_3 loss via leaching are the most crucial types of N loss in agricultural ecosystems and for this reason any effort that reduces the uncertainty around MPD parameters can lead to more robust model predictions (i.e. calibration using measured data).

The MPD parameters that had the strongest impact on simulated N_2O and NO_3 (i.e. AMAXX, EFFAC) represent difficult-to-measure aspects of the soil's biogeochemical processes. Deriving better estimates on the "true" value of these three parameters can come through (1) measuring the ratio of CO_2 to dissolved organic C (DOC) that is released during the decomposition of organic matter (for the EFFAC parameter) and (2) a measurements-based estimate of how resilient soil microbes are. Such measurements can be taken in a laboratory environment but are not possible in field conditions, which creates the need for identifying and measuring suitable proxies. In general, the fact that our knowledge about the dynamics of the soil's microbial population is rather limited, and mostly lab-based, has been widely recognised (Wang and Chen, 2012; Butterbach-Bahl and Dannenmann, 2011; Sutton et al., 2011). Our results, though specific to the Landscape-DNDC model, show that this lack of knowledge can be consequential in terms of model-based prediction of N_2O emisisons and NO_3 leaching.

It should be noted that the most important MPD parameter (i.e. EFFAC) strongly affect all of the examined outputs. This means that by modifying the values of this parameter the user can increase/decrease the size and reactivity of the soil's microbes, which will almost directly lead to increase/decrease in the N and C-based outflows (e.g. total annual CO_2, N_2O etc) from the system. However, altering this and other influential MPD pameters (e.g. AMAXX, microbial pool C:N ratio parameters) will not affect the temporal patterns of the various N and C-based outputs strongly because these patterns are mainly controlled by environmental conditions (e.g. precipitation events) and human management (e.g. fertiliser application dates).

The temporal patterns of the N-based outputs are particularly affected by the GPD group of parameters. This is mostly due to the fact that in Landscape-DNDC the soil is split into a user-defined number of layers of varying thickness. This soil discretisation by depth also means that the modelled processes (e.g. water, nutrient and gas movement) are calculated on a layer-by-layer basis. As a result, the presence of any N-based gas in a certain soil layer partly depends on how much gas was diffused into that layer. The fact that no single parameter appears to dominate the GPD group means that it is the combination of GPD parameters that defines the amount N-based outflows (e.g. N_2O, N2). While parameters that control gas production processes were shown to be important (e.g. KNIT, EFF NO_2), the model's few gas diffusion-related parameters are also playing a role (DNO, DN_2O) and so do parameters that relate the soil's physical structure to gas diffusion (i.e. EC parameters like EXP1 NX). In general, most of the GPD parameters are related to rather well-studied aspects of soil biogeochemistry (Butterbach-Bahl and Dannenmann, 2011).

The EC group includes parameters that describe the role of the soil's physical and chemical conditions on the various modelled processes. These are parameters for which our experiment-based understanding is quite extensive and EC parameters are essentially the quantitative interpretation of how we believe soil conditions relate to microbe-mediated nutrient transformations (i.e. mineralisation, immobilisation, decomposition) (Kesik et al., 2006). These parameters were found to be particulary important for the simulation of N uptake, soil C, NH_3 volatilisation and NO_3 leaching. The most important of the EC group of parameters were found to be those that link the soil's pH, temperature and moisture content with the decomposability of the soil's C and N substrate.

4.2. Edaphoclimatic conditions and time-dependency

The framework that was used to quantify the parametric sensitivity of Landscape-DNDC guaranteed that the final results are not biased by the edapho-climatic conditions of a single site. The SA was performed independently on three UK arable sites and produced exactly the same parameter ranking (i.e. S_T and S_i per output). This means that the edapho-climatic conditions in the three sites had a similar effect on the model's parametric sensitivity. However, this should not be considered as a universal observation and we believe that the use of more than one site should be part of SA studies (van Werkhoven et al., 2008). In particular, the use of field data from multiple sites in model sensitivity analysis (and calibration) should be considered as a prerequisite for the application of agroecosystem models at large spatial scales (e.g. sub-national). Following this approach is the only way to guarantee that the soil and climate conditions in a single agroecosystem have not lead to conclusions that are unrepresentative of the larger area.

In terms of the time-dependency of the estimated SIs our approach was simple and intended to demonstrate a method to obtain a measure of how temporally dynamic the influence of parameters is in relation to each examined output. The examination of the results of this analysis in more detail was beyond the scope of this study. However, this simple approach allowed us to notice that the sensitivity of certain outputs (e.g. NO_3 leaching and N uptake) should be examined on a weekly rather than an annual basis in order to avoid the risk of overlooking important parameters. Considering the fact that our output aggregation was based on the timing of fertiliser application we identified outputs whose parametric sensitivity is influenced by fertiliser addition either more weakly (i.e. soil C, microb population, mineralisation, nitrification) or more strongly (i.e. all other outputs but particularly NO_3, N_2O, NO and N uptake). In this context, we could also argue that the parametric sensitivity of outputs of processes that are simulated by the model first (e.g. allocation of C and N into modelled pools) shows a small time-dependence compared to processes that are simulated at later stages (e.g. gas production and diffusion through the soil).

4.3. Process-based agroecosystem BGC models

This study can serve as a guide to users of the Landscape-DNDC model who want to calibrate the model and/or want to quantify the parameter-induced uncertainty around its outputs (i.e. reduce parameters included in uncertainly analysis). Because the calibration of any number of model parameters will affect more outputs than simply the output of interest (typically a single output) it is important to have an understanding of which other outputs are particularly sensitive to the parameters that will be calibrated. In this context, this study provides a quantitative picture of the parametric sensitivity of key ouputs of Landscape-DNDC. Considering the similarities (i.e. conceptual, parameters and processes) between Landscape-DNDC and other DNDC-based models, the results of this study can be a starting point for future parametric SAs and calibration studies using other DNDC-based models.

While DNDC-based models are widely used to predict yields, soil C and greenhouse gas emissions there is a lack of studies on the parametric sensitivity of their outputs. We were unable to identify studies that focus on agroecosystems and examine the parametric sensitivity (full set of parameters) of a DNDC-based model. Rahn et al. (2012) presented the only study, to our knowledge, that considered the role the parameters on the predictions of Landscape-DNDC albeit focusing on forests and on model calibration against CO_2, NO and N_2O data. Among the 25 key parameters that were used in Rahn et al. (2012) we found most of the parameters that were identified as being important in our study. Qin et al. (2013) performed input SA analysis on the prediction of soil C, N_2O and wheat yieds by DNDC model and found that a small number non-weather input parameters affected the examined outputs significantly. In one of the few parametric sensitivity studies using a process-based agroecosystem BGC model, Necpálová et al. (2015) examined the sensitivity of soil C and N_2O predicted by the DayCent model. In agreement with some of our findings, Necpálová et al. (2015) found that only a few parameters affected the examined outputs noticeably while the impact of microbe-related parameters (i.e. parameters that would have been in our MPD group) was stronger in relation to N_2O prediction than it was in relation to soil C prediction, for which edaphoclimatic parameters played dominant role (i.e. parameters that would have been in our EC group).

5. Conclusions

This study showed that relatively few parameters control the parametric sensitivity of the outputs of Landscape-DNDC. Among them, the parameters that control the population and dynamics of soil microbes (MPD group) and those that link soil conditions (e.g. pH, temperature) to biogeochemical processes (EC group) are the prime causes of output sensitivity. The parameters that control the production and diffusion of gases in the soil (GPD), being the smallest in term of the number of parameters included, was proven to be particularly important for the prediction of greenhouse gas emissions. Because the different processes described in the model have been studied in varying extends we argue that focusing on reducing the uncertainty around the MPD parameters represents a well-grounded way to improve the quality of the model's outputs and its overall performance. Moreover, our comparison of the annual-based and the weekly-based SA results showed that there are variables for which the list of important parameters can change considerably when the temporal resolution of the outputs changes from being a whole year to being one or more weeks. This fact highlights the role played by the temporal resolution of the outputs used in SAs and should be considered as a model-independent observation.

We believe that the systematic approach to SA presented in this study offers two advantages compared to simpler approaches. Firstly, role-based grouping of model parameters makes the results of sensitivity studies more understandable and easy to communicate while it can be particularly useful when deciding where to focus model calibration (i.e. which processes and related parameters). Secondly, the comparison of the weekly-based against the annually-based SA results, while not exhaustive, adds to the validity of the conclusions of an SA study. In this context, we argue that SA studies of agroecosystem BGC models should take into account the fact that time-dependency of the sensitivity indices for certain types of outputs (e.g. greenhouse gas emissions) can be significant and therefore should be considered explicitly. Finally, we suggest that SA studies on agroecosystem models would be more robust if, as was done here, the simulations are performed in more than one site in order to ensure that the role of ecosystem heterogeneity is considered.

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Appendix

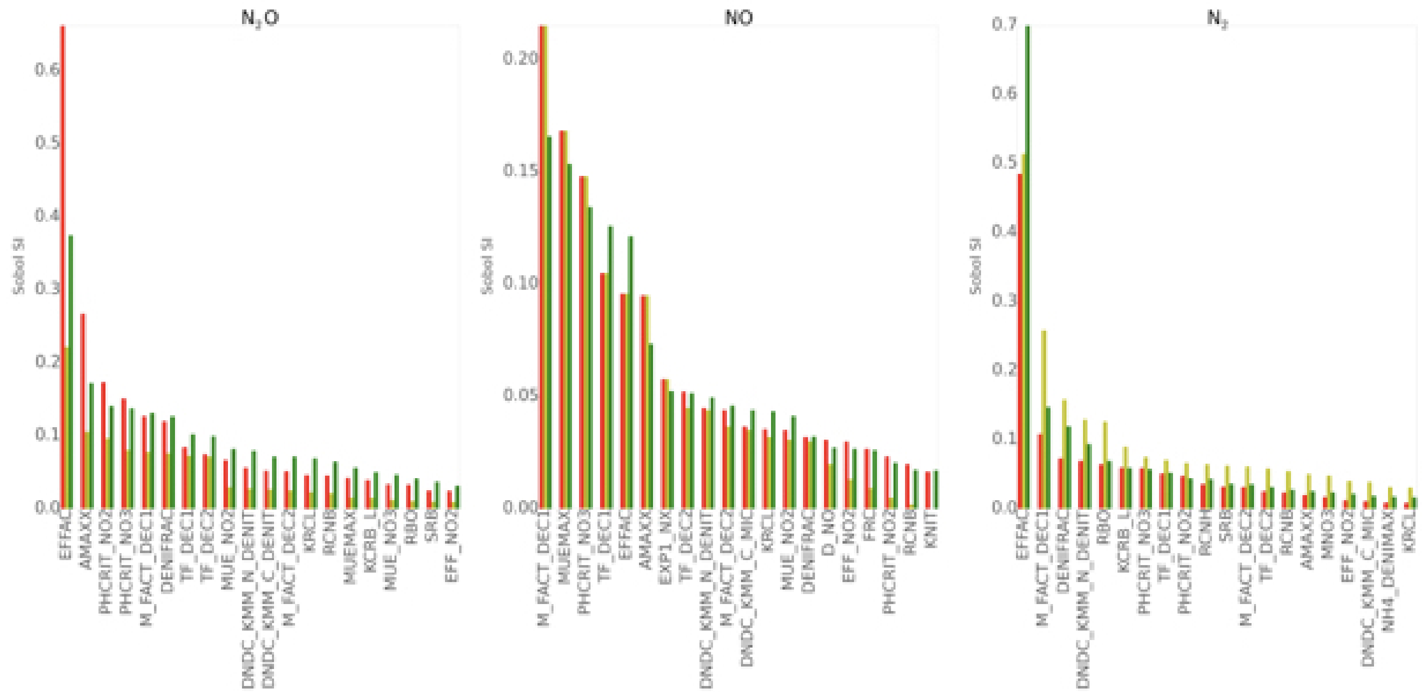

Figure 5: Sobol total (S_T) sensitivity indices (20 most important parameters) for N_2O, NO and N_2. Red: Edinburgh, Yellow: Gleadthorpe Green: Terrington

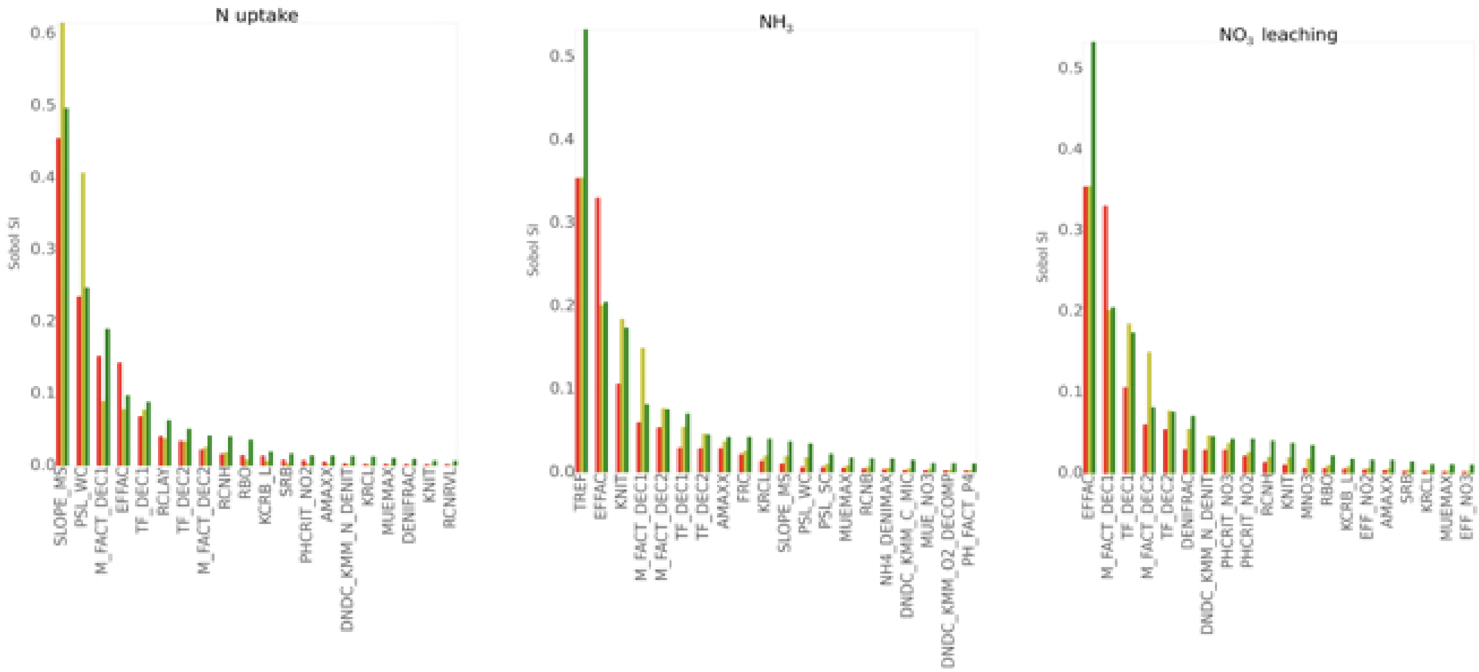

Figure 6: Sobol total (S_T) sensitivity indices (20 most important parameters) for N uptake, NH_3 and NO_3 leaching. Red: Edinburgh, Yellow: Gleadthorpe Green: Terrington

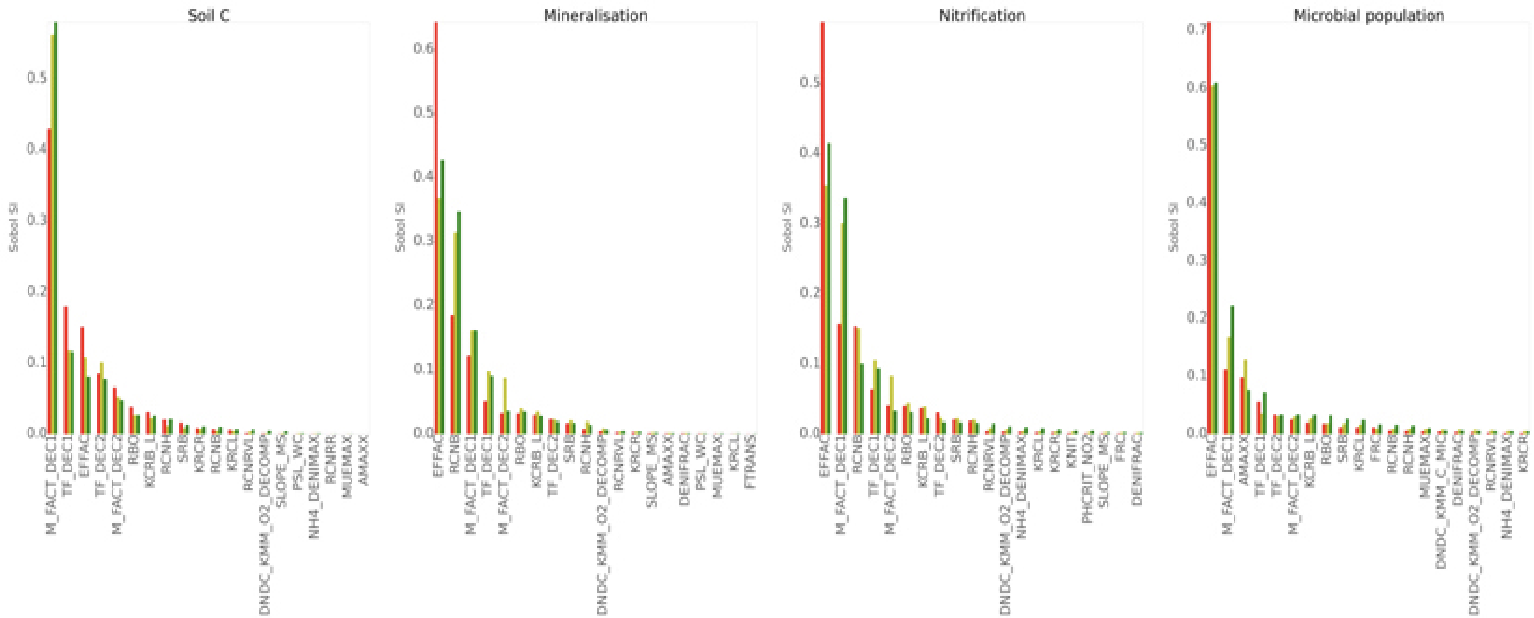

Figure 7: Sobol total (S_T) sensitivity indices (20 most important parameters) for soil C, mineralisation, nitrification and microbial population. Red: Edinburgh, Yellow: Gleadthorpe Green: Terrington